Application of Spectroscopic Methods in Molecular Structure Determination

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Lecture - 35

Structure solving based on IR, UV-Vis, MS, 1H and 13C NMR Spectroscopic data

Problem solving session

Hello, welcome to the course on Application of Spectroscopic Methods in Molecular Structure Determination. We will wind up the course with couple of problem solving sessions. In this problem-solving session, will try to identify organic molecules, the structure of organic molecule based on multiple spectroscopic data namely infrared, UV visible, mass, proton, carbon 13, NMR spectroscopic data.

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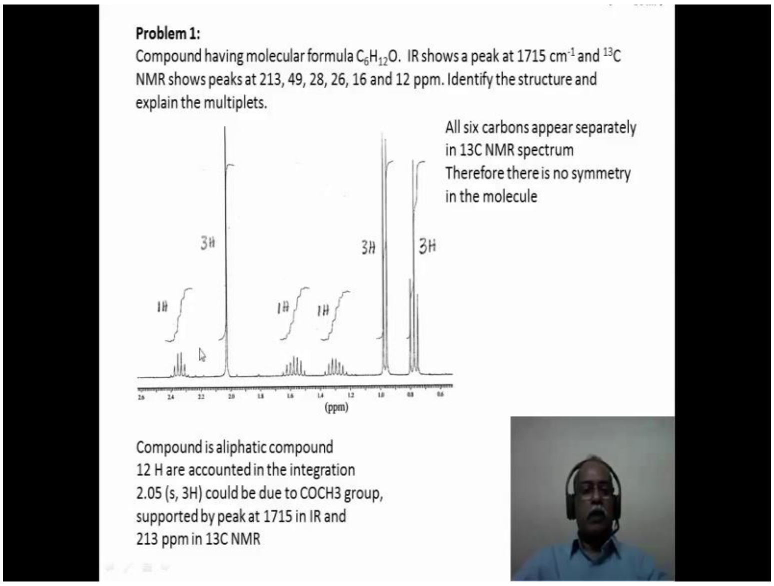

Problem 1:

Compound having molecular formula $C_6H_{12}O$. IR shows a peak at 1715 cm^{-1} and ^{13}C NMR shows peaks at 213, 49, 28, 26, 16 and 12 ppm. Identify the structure and explain the multiplets.

All six carbons appear separately in 13C NMR spectrum
Therefore there is no symmetry in the molecule

Compound is aliphatic compound
12 H are accounted in the integration
2.05 (s, 3H) could be due to COCH3 group, supported by peak at 1715 in IR and 213 ppm in 13C NMR

In doing so, we will try to approach the problem in a logical manner, so that we can identify the structure of the organic compound based on the spectroscopic data that is given. A logical deduction of the structure is the most important point that i would like to emphasize in this problem solving session. The first problem is given here, the compound has a molecular formula of C6H12O. It shows an IR peak at 1715 inverse centimeter and there are 6 carbons signal starting from 213 all the way down to 12 ppm. We need to identify the structure of the compound. This figure is the proton NMR spectrum of this particular compound. We can see here, there are 3 hydrogen intensity, 3 hydrogen intensity, 3 hydrogen intensity, there are 3 signal totally 9 hydrogen. Then for 1 hydrogen intensity there are 3 singles, so 3 plus 3 plus 3, 9, 9 plus 3, 12 hydrogen's. So all the hydrogen's are taken care of accounted for (Refer Time: 01:30) integration, which corresponds to the heat C6H12 the 12 hydrogen's are taken care of the in the integration.

Now, right away you can tell that, this is an aliphatic compound because the spectrum consists of peaks only from 0.6 ppm to about 2.6 ppm. There are no signals, about 2.6 ppm in this compound and hence the region about 2.6 is not displayed here. Therefore, we conclude the conclusion the compound is aliphatic and it is probably a saturated aliphatic compound there are no carbon carbon double bonds or there are no aromatic ups in this particular structure. Now, there is a signal at 2.05 which is a singlet of 2 hydrogen intensity because it is aliphatic compounds. We can conclude that it is a COCH3 kind of a group, which is further supported by the fact that you have a carbonyl peak at 1715, which is a saturated carbonyl compound peak and also there is a peak at 213, which corresponds to the carbonyl region in the carbon 13 NMR spectrum of this compound.

Now, what is important is there are 6 carbons in the molecular formula and there are 6 peaks in the carbon 13 spectrum that means, this molecule does not possess any kind of a symmetry, so the number of signals that you see corresponds to the number of carbon that is present in the molecule. If it were a symmetrical molecule the number of signal would have been reduced such is not the case in this particular example, so the molecule possess no symmetry elements as it is. These multiplets are expanded for the sake of convenience to see their nature of the multiplet. The first multiplet at around 2.38 or so is expanded here and one can clearly see that it is a 2.34 signal which is line 1, 2, 3, 4, 5, 6 there are 6 lines here

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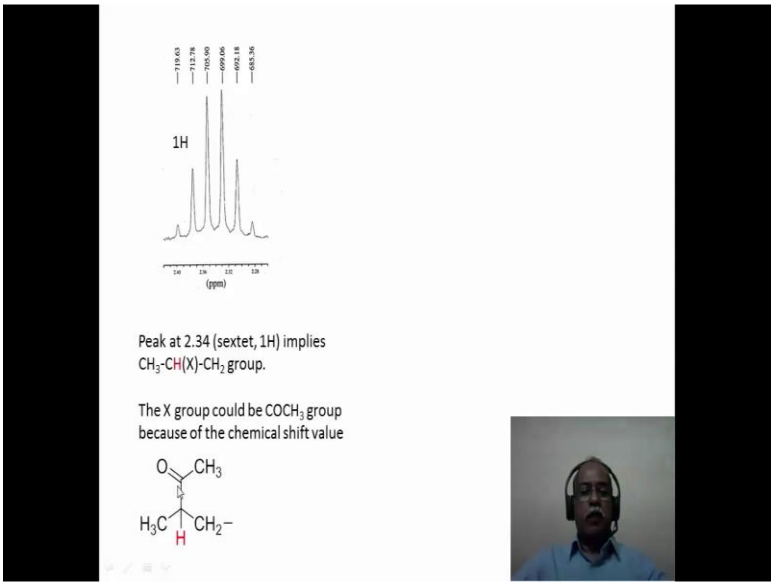

Peak at 2.34 (sextet, 1H) implies CH_3-CH(X)-CH_2 group.

The X group could be $COCH_3$ group because of the chemical shift value

It is a sextet of 1 hydrogen intensity. It simply implies there are 5 hydrogen’s adjacent to this CH kind of a group and CH is attached to an X and recent, we say CH is attached to an X's because of the chemical shift is around 2.32. X could be the acetyl group so when it acetyl is attached to the CH group here that would correspond to somewhere around 2.3, 2.4 in that region. This CH which is indicated in the red color is surrounded by a CH 3 and CH 2 group. There are totally 5 hydrogens on the adjacent carbon and hence sextet is obtained for this particular signal. Now, one can calculate the coupling constant value because the frequencies of the 5 lines are already printed out here, so if you subtract 716.63 from 712.78 it get roughly 6.9 hertz or so.

The coupling constant is approximately 6.9 hertz in this particular case which of course, corresponds to the average vicinal coupling constant that one would expect in an aliphatic chain of this kind. So, we come to the conclusion based on this logical argument that this hydrogen which is a red color indicated hydrogen is a sextet because there are 5 hydrogen’s adjacent carbon and the X group is corresponding to the acetyl group. We came to the conclusion that there is an acetyl group based on the fact that there is a singlet in the NMR spectrum around 2.205. We used that acetyl group to account for the chemical shift value which is corresponding to 2.6 2.3 4 or so in this particular case which would be an ideal chemical shift value for the CH functional group.

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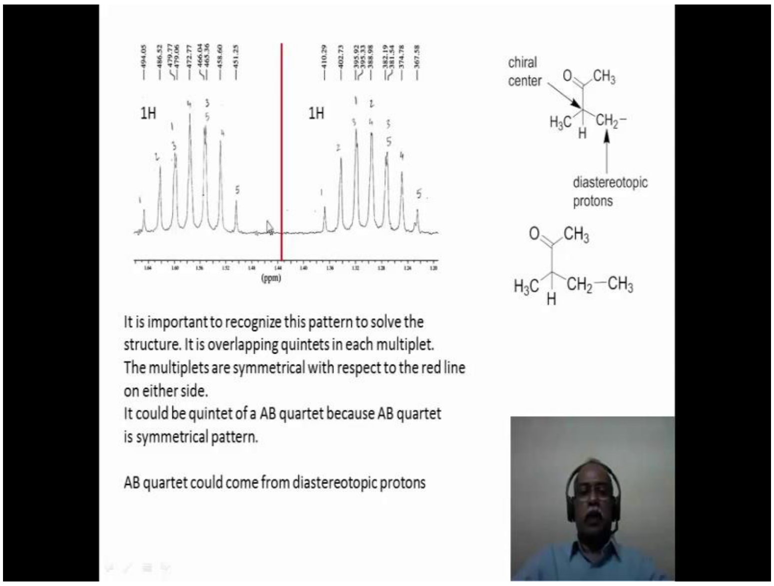

It is important to recognize this pattern to solve the structure. It is overlapping quintets in each multiplet.
The multiplets are symmetrical with respect to the red line on either side.
It could be quintet of a AB quartet because AB quartet is symmetrical pattern.

AB quartet could come from diastereotopic protons

Now, this is a complex multiplet is what is shown here in the NMR spectrum. If you see this region between 1.2 and 1.7 is expanded and what is important in this region is that you can see symmetry with respect to the red line that is shown here. If the red line were to be a mirror plane 1 half of the spectrum is reflected in the other side of the mirror plane, so if you have a mirror image symmetry relationship with this particular multiplet and the multiple each one has the 1 hydrogen intensity in terms of the signal intensity corresponding to that. This would mean that there is a possibility to assume that this is a multiplet corresponding to about 10 line pattern on this side and 10 line pattern on this side I will count the number of lines for you, this is line 1, line 2, line 3, line 4 and line 5 and then again there is a line 1, line 2, line 4 and line 5.

In other words this is a overlapping quintet kind of a system is what we have. So, overlapping quintet will have 10 lines, some of the lines are merged on top of each other and that is why you do not see it. Similarly, here also it is a overlapping quintet so what would have happened is this possible that there was an AB quartet and the AB quarter is further split into a quintet by means of a coupling between the 2 hydrogen’s first. The AB quartet comes from a diastereotopic type of hydrogen, so if we have for example this particulars fragment which we have already identified, this carbon is a chiral carbon, so this CH 2 here is a diastereotiopic hydrogen no matter what group you are attaching in this particular position. Because, this is a diastereotiopic hydrogen, this would appear has a symmetrical AB pattern.

If it is further split into a quintet then the structure must be like this, you have 4 hydrogen’s which are adjacent to the CH 2 hydrogen, so the CH 2 hydrogen will coupled with each other first of all to form a AB quartet and the AB quartet will be further split into a quintet, so AB quartet times quintet will be 20 line pattern. There are 10 lines on this which are overlapping with each other, there are 10 lines on this multiplet also which are overlapping with each other. It is important to identify or recognize this particular pattern to solve this structure. The overlapping quintet in each multiplet is what is to be recognized in this particular multiplet kind of a signal.

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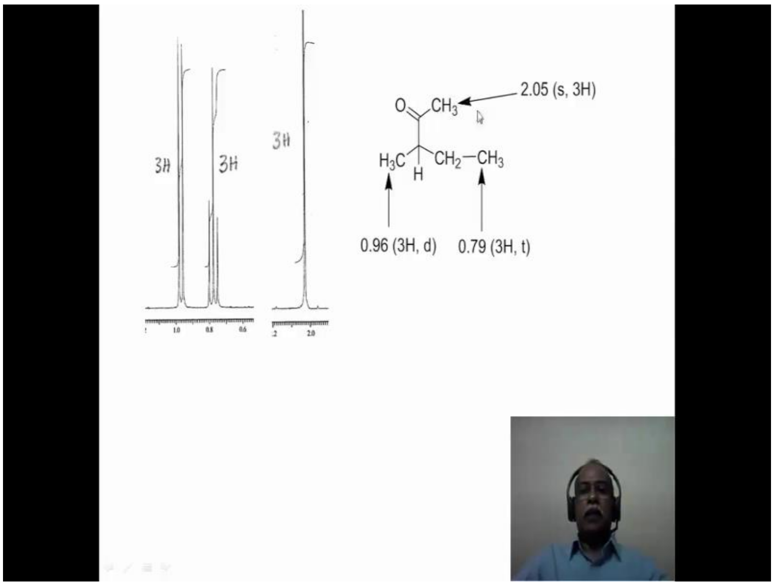

Then you have 3 hydrogen intensity signal which are specified here, now this structure is more or less confirmed from the fact that you have this pattern which would only correspond to a CH 3 group being attached and this of course corresponds to the molecular formula C6H12O and takes care of the molecular formula also. So, 1 can now easily assigned the rest of the multiplet.

This particular hydrogen will split this methyl into a doublet, so that methyl comes as a doublet around 0.96 ppm or so in this region here this corresponds to a 3 hydrogen intensity. And this CH 3 will be split into a triplet and that triplet is very clearly seen around 0.79 ppm or so. Finally, this singlet already we have seen that it appears as a singlet because there are no coupling partners associated with this.

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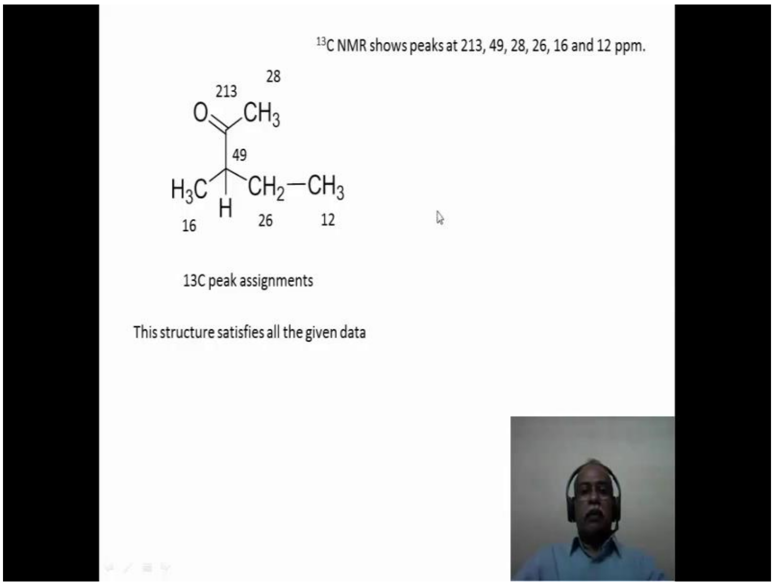

^{13}C NMR shows peaks at 213, 49, 28, 26, 16 and 12 ppm.

13C peak assignments

This structure satisfies all the given data

The carbon 13 can be easily assigned. The carbonyl carbon will have the highest frequency 213 and then comes the methine hydrogen which is as a lot of substituents it is 49, then comes this CH 3 which is attached to the CO that will be around 28 and the rest of the carbon will have a higher chemical shift and the terminal carbons will have the lowest chemical shift finally. So, the structure essentially satisfies all the given data and hence we solve the structure in the logical manner here of course, one does not have the mass spectral data only IR data, NMR data is given and based on these 2 data we are able to solve the structure of this particular molecule this case.

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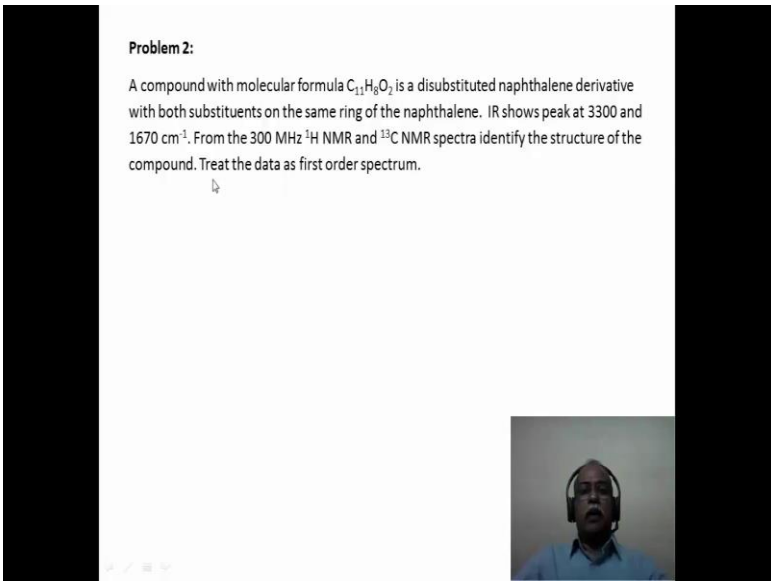

Problem 2:

A compound with molecular formula $C_{11}H_8O_2$ is a disubstituted naphthalene derivative with both substituents on the same ring of the naphthalene. IR shows peak at 3300 and 1670 cm^{-1}. From the 300 MHz ^{1}H NMR and ^{13}C NMR spectra identify the structure of the compound. Treat the data as first order spectrum.

Let us move on to problem number 2. The compound has a molecular formula as C 8 H C11H8O2 and it is already mention that it is a disubstituted naphthalene derivative in which both the substituents are on the same ring of the naphthalene. In other words the problem amounts to identifying the 2 substitutents that are present here and placing them appropriately on the naphthalene ring on one particular aromatic ring, both the substituents are present. The IR shows peaks at 3300 inverse centimeter and 1670 inverse centimeter. This would indicate that there is OH kind of a hydrogen, one can confirm both in the IR spectrum 3300 inverse centimeter.

One can also look at the NMR spectrum and see whether they are exchangeable hydrogen’s in the NMR spectrum. 1670 of course, would be that is an alpha beta unsaturated carbonyl system, this is a every characteristic region for a alpha, beta unsaturated carbonyl. So, from the proton NMR and carbon 13 NMR, one need to identify this compound and it is given that treat all the data as a first order spectrum. In other words the proton NMR spectrum can be treated as a first order spectrum.

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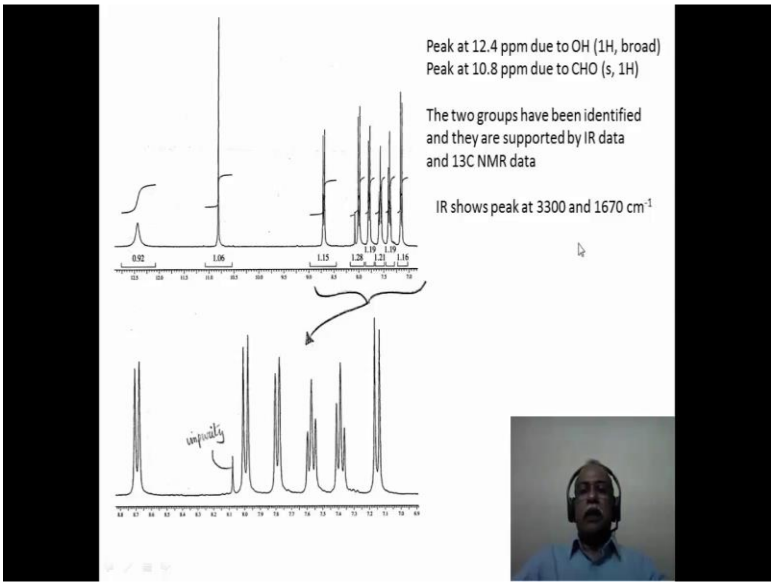

Peak at 12.4 ppm due to OH (1H, broad)
Peak at 10.8 ppm due to CHO (s, 1H)

The two groups have been identified
and they are supported by IR data
and 13C NMR data

IR shows peak at 3300 and 1670 cm^{-1}

This is a proton NMR spectrum of this compound. We can see here from 7 ppm to about 12.5 ppm or 13 ppm range is what is given, that means there are no aliphatic side chains attached to the naphthalene ring. There is a peak at 12.5 or so which is having a very high chemical shift value and it is also broad, this is probably because of an OH kind of a hydrogen that is present in this system. 1 hydrogen intensity broad signal would correspond to an OH kind of a system. Then you have another signal around 10.8 or so this is also a singlet of 1 hydrogen intensity, this is a very characteristic region for the aldehyde functional group.

So, we have identified both the functional group 1 has the hydroxy functional group and other one has a aldehyde functional group and the expansion of the multiplet in this region between 7 to 9 ppm is shown here with this peak being marked as an impurity peak (Refer Time: 11:18) comes from not from this compound, but some other impurity is being present in the system. IR shows 3300 and 1670 and that would essentially confirm the fact that you have a OH which will correspond to the 3300 and you have the CHO which would correspond to the 1670 kind of a peak in the NMR spectrum, aldehyde is corresponding to the 10.8 ppm which is corroborated in the IR spectrum by the peak at 1670 inverse centimeter or so.

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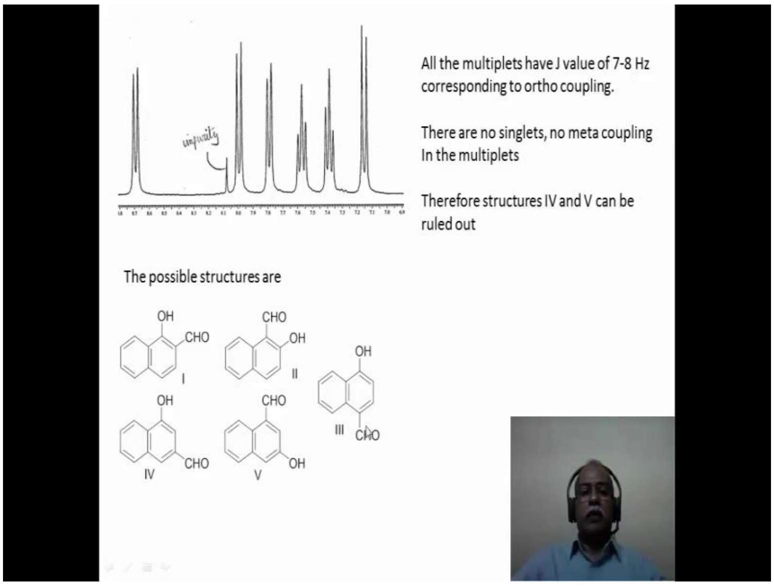
All the multiplets have J value of 7-8 Hz corresponding to ortho coupling.

There are no singlets, no meta coupling In the multiplets

Therefore structures IV and V can be ruled out

The possible structures are

Now, what is important to recognize in this particular spectrum is that each one of this multiplet, that is this multiplet here there is a doublet, there is doublet, triplet, triplet and a doublet. All of them have 1 hydrogen intensity in terms of the integration of the signal. If it is a disubstituted naphthalene you should have 6 protons present here, this is proton 1, 2, 3, 4, 5, 6 there are 6 signals where are very clearly seen in the NMR spectrum. What is even more important is that each one of these multiplet has J value of about 7 to 8 hertz or so which corresponds to the ortho coupling. One can take the gap between this 2 multiplet and calculate the frequency. The frequency is 300 megahertz NMR spectrum this is very clearly given in the beginning. So, 1 ppm would correspond to 300 hertz or so, in other words from 7 ppm here all the way up to 8 ppm this length would be essentially 300 hertz so 1 can find out what is the gap between these 2, how many hertz it belongs to and so on.

I have done this exercise and each one of the multiplet corresponds to about 7 to 8 hertz or so which would corresponds to ortho coupling in this case, that means there are no meta coupling in the multiplet, so 1 can rule out the possibility that you have as the compound structure 1, structure 2, 3, 4, 5 these are the possible structures that 1 can have where the aldehyde functional group and hydroxy functional group are put on the same ring of the naphthalene unit. Structure 4 and 5 can be easily ruled out because this particular hydrogen which is adjacent to the aldehyde and the hydroxy peak that would not have any kind of an ortho coupling partner. Since all the peaks are having ortho couple kind of a J value, this 2 structures which will not have an ortho coupling for this particular hydrogen can be easily ruled out.

On other words, this hydrogen which is adjacent to the aldehyde and the OH and this hydrogen which is adjacent to the OH in this case and adjacent to the aldehyde in the case of compound 4 cannot be a multiplet with the ortho coupling. So, compound number 4 and 5 essentially are ruled out based on the fact this does not bare the (Refer Time: 14:01) coupling constant in terms of the ortho coupling being absent for these 2 hydrogen’s that are mentioned in this particular range. It aboils down to identifying compound 1, 2, 3 for this particular structure in this case.

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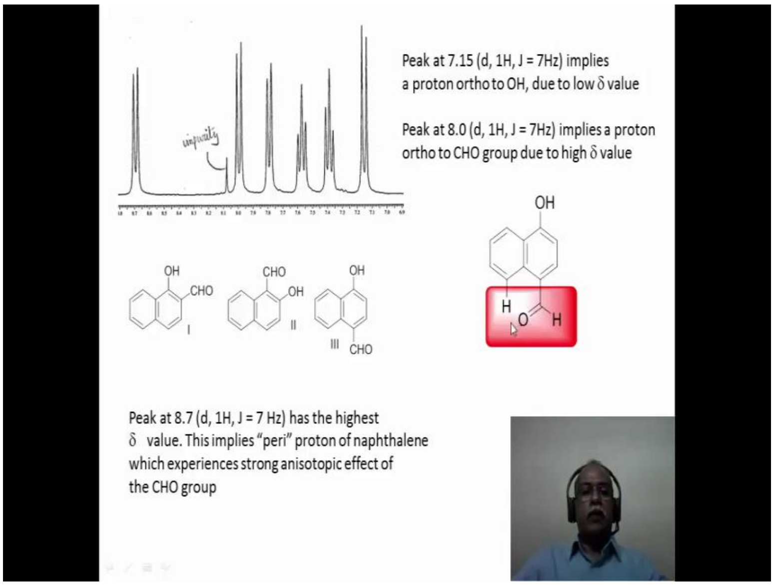

Peak at 7.15 (d, 1H, J = 7Hz) implies a proton ortho to OH, due to low δ value

Peak at 8.0 (d, 1H, J = 7Hz) implies a proton ortho to CHO group due to high δ value

Peak at 8.7 (d, 1H, J = 7 Hz) has the highest δ value. This implies “peri” proton of naphthalene which experiences strong anisotopic effect of the CHO group

So, now if you start to analyze this peak at 7.15 which is this doublet here which is 7 hertz coupling implies there is a proton ortho to oh because this is a very low chemical shift value. Benzene is around 7.3 when you attach a hydroxy functional group, the phenolic compounds proton NMR would be less than 7 hertz or so this is coming around 7.15 hertz, so it must be a adjacent to an ortho to the hydroxy functional group. One can for example, rule out this structure because it does not have any ortho hydrogen adjacent to the hydroxy functional group, so compound one can be ruled out.

Compound 2 and 3 has adjacent hydroxy group to the ortho to the hydroxy functional group, so they can be retained. Peak at 8 ppm which is this particular peak again is a doublet, it implies there is a proton adjacent to the CHO group. So, we can assume that this is a compound structure based on this information, this can be further confirmed by the fact that there is a peak at very high delta value which is about 8.7 ppm or so and this would imply that there is a peri hydrogen which is experiencing an anisotropic effect of the aldehyde functional group. What I mean is, if you take this hydrogen which is the peri position of the naphthalene there is an aldehyde group which is in the other peri position of the naphthalene because of the anisotropic effect of the aldehyde functional group or any carbonyl functional group in the peri position will effect this particular hydrogen and push it to very high delta value of around 8.8 or 8.9.

This information may not be known to you, but please bear in mind that whenever you have an aromatic compound which have signals above 8.5 ppm it is because of this kind of a strong anisotropic effect particularly of the peri type of this kind of compounds will result in a very high delta value of this thing. So, the anisotropic effect experienced by the peri hydrogen because of the formyl group which is the aldehyde group is responsible for this particular peak here.

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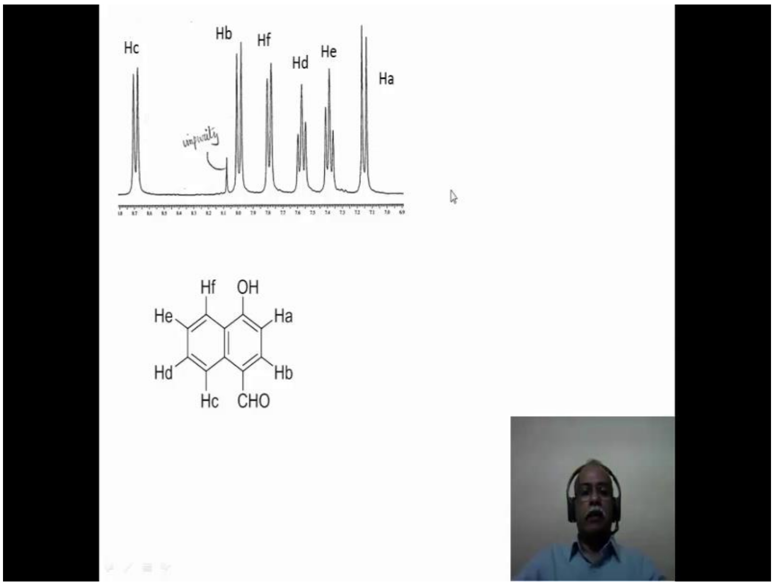

So, one can come to the conclusion that this is probably most likely structure for this particular compound and the proton NMR is very clearly assigned, the Ha which is adjacent in to the hydroxy functional group or ortho to the hydroxy functional group comes has the lowest delta value and it is a ortho coupling with Hb, so Ha and Hb are mutually coupled, so Ha comes here and the Hb most likely is this particular peak which has the same coupling constant. In other words, these to form an AB quartet one half of the ab quartet is here, the other half of AB quartet is around 7.15 ppm or so. Now, in the other ring you have 4 hydrogen Hc, Hd, He and Hf. Let us take Hd and He, Hd has 2 adjacent ortho hydrogen so that would ortho couple with each of the hydrogen and if the ortho coupling constants are accidentally same Hd would appears as a triplet. In fact, there are 2 triplets here both He as well as Hd will appear as a triplet.

This one that is corresponding to Hd and this one is corresponding to He and this is essentially based on the electronic effect that would be more in the case of Hd compared to the electronic effect of the aldehyde which will be less in the case of the He. So, He is more shielded compared to Hd which is more deshield in this particular case. Finally, we are left with Hc and Hf which have only 1 ortho coupling partner He and f will couple with each other, so He and Hf doublet because of the absence of any electronic peri effect in this particular case. Hc comes a highest delta value in the NMR spectrum.

Essentially, this structure satisfies the multiplicity that one experiences in the NMR spectrum and hence this probably is the correct structure.

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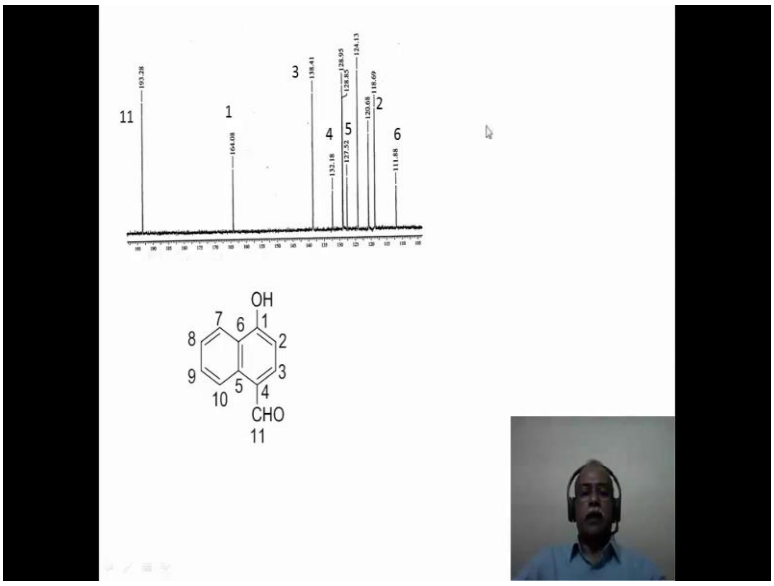

One can also assigned the carbon 13 spectrum H 11 which is the aldehyde hydrogen comes at 193 ppm or so. Then comes the carbon which is ipso to the oxygen. Oxygen is an electron withdrawing functional group it is directly attached oxygen this carbon that normally comes between 150 to 165 ppm, 164 ppm would correspond to carbon number 1 and carbon number 4 would correspond to this particular signal which is the less intensity this is a quaternary carbon, this is also a quaternary carbon. There are 3 quaternary sorry there are 4 quaternary carbons, carbon 1, carbon 4, carbon 6 and 5 so these less intense peak can be assigned to the quaternary carbon. The more intensity peaks can be assigned to the carbon bearing the CH.

So, using that logic 1 can assign 1 and 4 to peak number 1 and 64 ppm and 132 ppm. Peak 5 and 6 can be interchanged this is adjacent to ortho to the hydroxy functional group that is why I have put 6 as lowest delta value and 5 at a higher delta value around 127, 6 at 120 sorry 111 ppm or so. The 6, 7, 8, 9 peaks can be arranged between the CH peaks that are seen here, it is difficult to precisely arrange which one is 7 and which one is 8 among the peaks. What is important is, there are 4 CH carbons in this ring. All the 4

CH carbons are very clearly seen in the carbon 13 spectrum of this particular compound.

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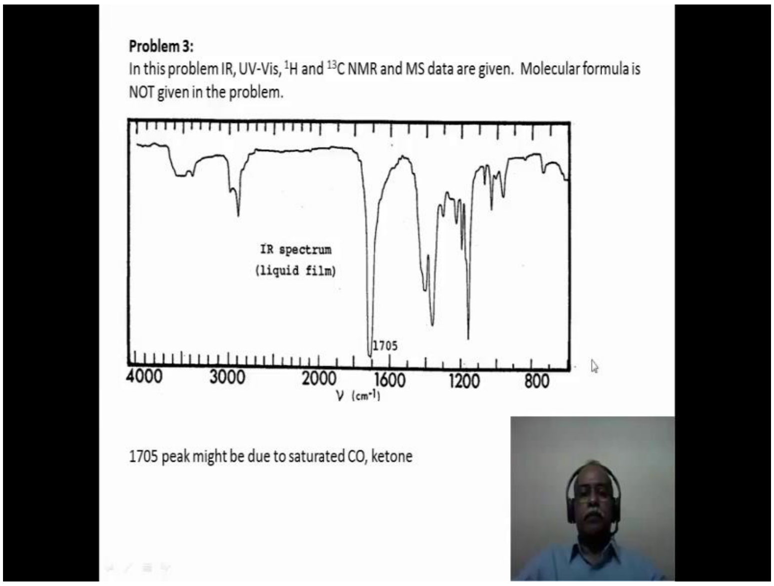

Problem 3:

In this problem IR, UV-Vis, ^1H and ^{13}C NMR and MS data are given. Molecular formula is NOT given in the problem.

1705 peak might be due to saturated CO, ketone

Now, let us move on to problem number 3. In this problem, the IR spectroscopic data, the UV visible spectroscopic data, the NMR data as well as the mass spectral data as given, however the molecular formula information is not given in this problem. So, one has to deduce the molecular formula also from the spectroscopic data that is given. This is a infrared spectrum of this compound and the only discernible peak that we can see for sure is the 1705 peak which would correspond to a saturated ketone kind of a system in this particular case. All the other peaks can be tentatively assigned, but 1 cannot confirm the only confirmatory information that 1 can get from the IR spectrum is that it is a carbonyl compound. What you see here is essentially because of adventitious water or something present gives this broad peak, it was truly a hydroxy compound it would be a very intense peak not a small peak like this. This is most likely due to atmospheric moisture or some such thing in sample.

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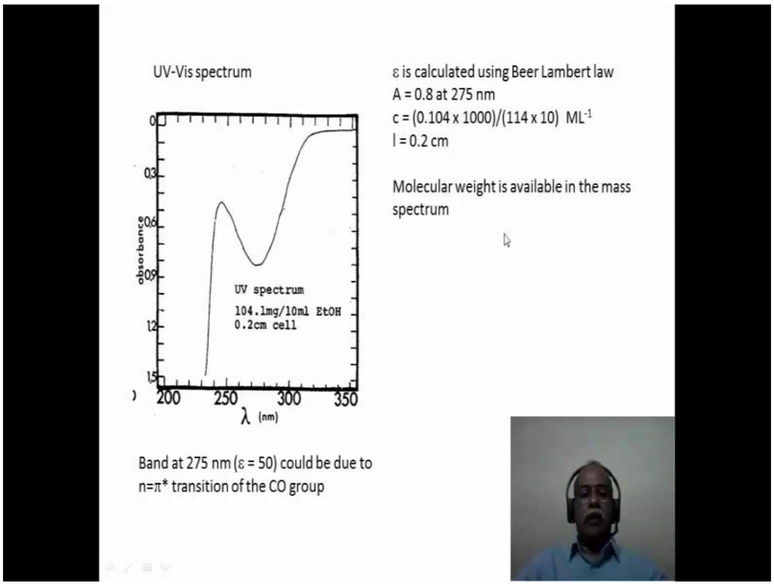

UV-Vis spectrum

ε is calculated using Beer Lambert law
A = 0.8 at 275 nm
c = (0.104 x 1000)/(114 x 10) ML^{-1}
l = 0.2 cm

Molecular weight is available in the mass spectrum

Band at 275 nm (ε = 50) could be due to n=π* transition of the CO group

This is a UV spectrum, for the first time we are trying to analyze UV spectrum in this module. There is a band that 275. In fact, the UV spectrum is plotted upside down, this is 0 value of absorbance and this is 1.5 value absorbance. Usually starts 0 from here to go up in the career, go up in the scale of absorbance. In this particular case it is reverse, so 1 has to read the spectrum in a top to bottom type of a reading.

The 275 nanometer peak has an epsilon as 50. How did I calculate the epsilon of 50? The concentration is given as 104.1 milligram per 10 ml which would correspond to 0.14 gram per 10 ml is the concentration. So moles per liter is calculated as 104 milligram multiplied by 1000 that is for the liter divided by the molecular weight, the molecular weight is given in the mass spectrum of this compound, so we know the molecular weight of this compound. The path length is shown as 0.2 centimeter the absorbance is taken as 0.8 corresponding to 275 nanometer.

Using the Beer Lambert's law, one can easily calculate the epsilon value which turns out to be approximately 49. something so I rounded it up to 50 epsilon mole inverse liter centimeter inverse is the unit that one can use for the epsilon value. Because it is a forbidden transition and it is a carbonyl compounds most likely this is because of the n pi star transition of the carbonyl system. Beyond that we do not have any kind of an information that can be gathered from the UV visible spectro. The UV visible spectrum is sort of ascertains are confirms the fact that it is a carbonyl compound by the presence of the n pi star peak being seen in this particular spectrum.

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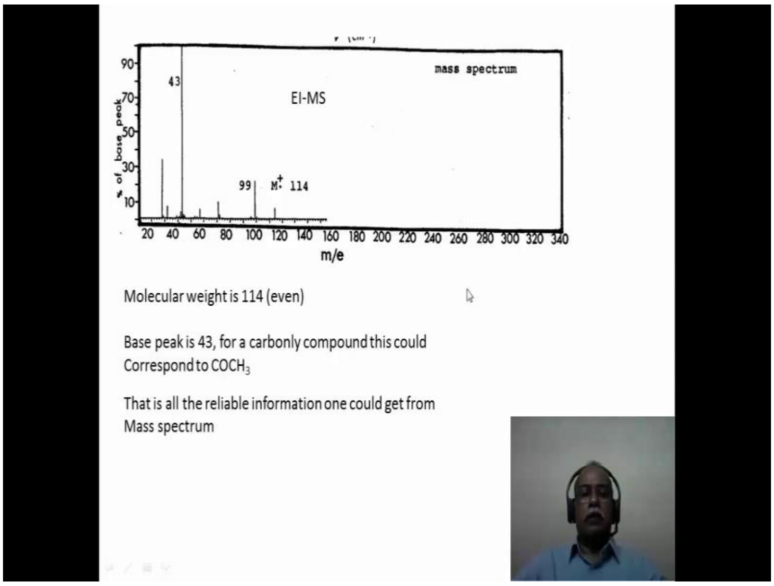

Molecular weight is 114 (even)

Base peak is 43, for a carbonly compound this could Correspond to $COCH_3$

That is all the reliable information one could get from Mass spectrum

This is the mass spectrum of the compound, it is an electron impact ionization mass spectrum of the compound. The molecular ion is seen as weak peak which is corresponding to 114, so this is a even number molecular weight you can be sure now that there is no nitrogen at least there is no odd number of nitrogen in this particular compound. The only other peak that we see very intense peak is the 43 peak. The 43 peak could correspond to the CH 3 CO group the acetyl group because it is a carbonyl compound it is most likely an acetyl group and that is a base peak in this particular spectrum. This is all the reliable information that one can get from the mass spectrum that is the molecular weight of the compound, molecular ion peak and the 43 peak which might be corresponding to the acetyl kind of a functional group in this system.

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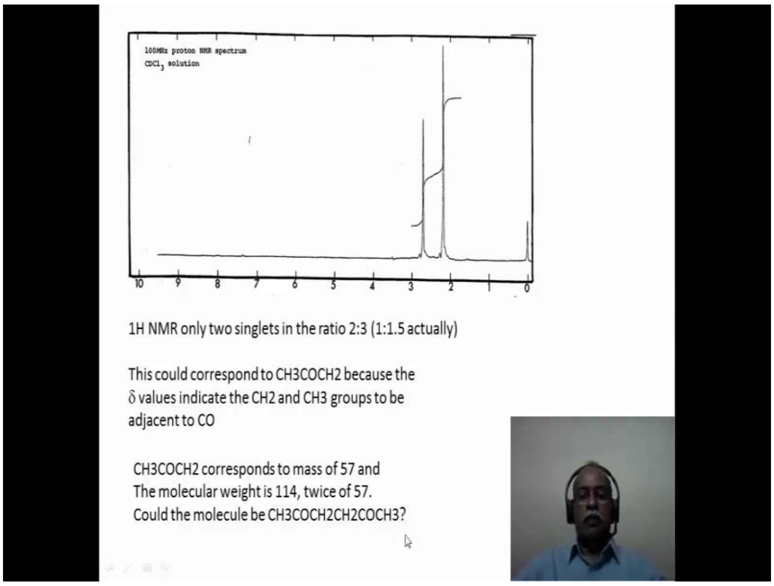

1H NMR only two singlets in the ratio 2:3 (1:1.5 actually)

This could correspond to CH3COCH2 because the δ values indicate the CH2 and CH3 groups to be adjacent to CO

CH3COCH2 corresponds to mass of 57 and
The molecular weight is 114, twice of 57.
Could the molecule be CH3COCH2CH2COCH3?

This is a proton NMR spectrum, again a very very simple spectrum in fact, if wonder whether you can get any kind of an information from this kind of a spectrum one can get an information. The integration first of all it is 1 is to 1.5 ratio, if this take this as 1 this would be 1.5. So, it must be actually 2 is to 3 or 4 is to 6 kind of a ratio is what should be present in the system. The NMR shows only 2 singlet, 1 singlet appearing around 2.05 ppm or so, the other signal appearing around 2.9 ppm or so. This could correspond to a CH3COCH2 kind of a functional group, because of the chemical shift value this 2 hydrogen’s of this signal here and the 3 hydrogen of this signal should be adjacent to a carbonyl functional group.

We already have evidence in the mass spectrum as well as in the infrared spectrum for the presence of the acetyl group for example. Most likely, this is the fragment that would correspond to the NMR signal that is seen here. What is important is the CH3COCH2 corresponds to a mass unit of 57, the molecular weight of the compound is 114 which is about twice of the 57. So, it is possible that this molecule is actually CH3COCH2 times, 2 times that would account for the molecular weight of 114 and being a symmetrical molecule it will also account for the proton NMR spectrum. For example, these 2 Ch two's are identical now so that will only give a singlet and the terminal CH three's are also identical because the molecule is symmetric with respect to the central carbon

carbon bond. That would also give a integration of singlet corresponding to integration of 6 hydrogen. So, 1 is to 1.5 ratio actually is 4 is to 6 ratio in reality, this formula or this structure of the compound were to the correct structure of the compound.

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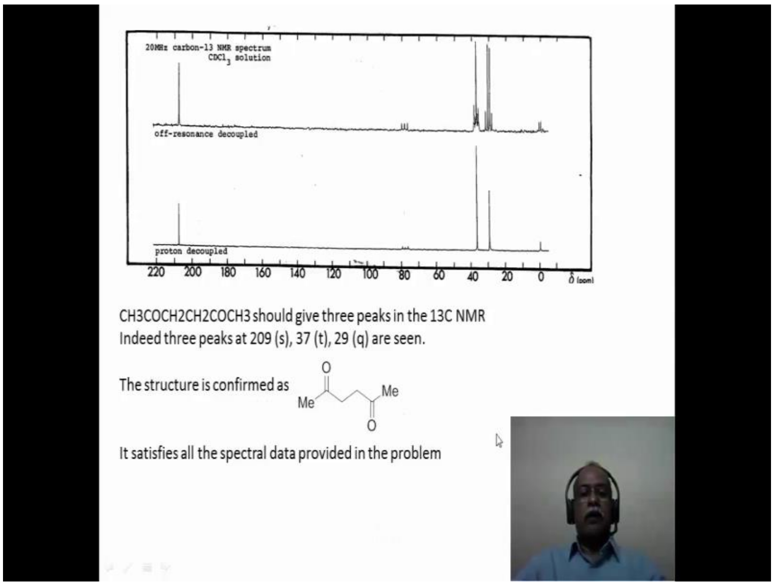

CH3COCH2CH2COCH3 should give three peaks in the 13C NMR
Indeed three peaks at 209 (s), 37 (t), 29 (q) are seen.

The structure is confirmed as

It satisfies all the spectral data provided in the problem

And let us see if the carbon 13 also supports this notion. This molecule being a symmetrical molecule you should see only 3 signals in the carbon 13 spectrum. This CH3COCH2 is the signals that one need to see, in fact CO is see in around 209 ppm or so as a singlet in a off resonance spectrum would should correspond to a ketonic compound. Then comes the peak around 38 ppm or so which would correspond to the CH 2 which is a triplet in the off resonance spectrum. The terminal CH 3 comes around 29 ppm or so which is a quartet in the off resonance spectrum. These 3 lines that you see is because of the cd cl 3 signal, it is because of the solvent carbon is coming around the 77 ppm or so. So the structure that is shown here which is actually 1, 2, 3, 4, 5, 6 hexa 2 5 dione is the correct structure of the compound.

In fact, all the spectral data can be explained on the basis. Mass spectrum is essentially fragmentation corresponding to this fragment will give you the acetyl peak or fragmentation corresponding to this particular bond breaking will give the acetyl peak being a symmetrical compound. If it breaks in the middle essentially it will give the half the molecular weight, molecular ion peak is very clearly seen in this particular case. We are actually deducing the structure of this compound even without the molecular formula information.

What is essential or crucial in the spectrum is the identification of this particular fragment and recognizing the molecular weight of this fragment is a exactly corresponding to half the molecular weight of the compound from the mass spectrum. Mass spectrum tells you the molecular weight to be 114, this fragment is 57, so it should be twice this fragment which would correspond to the structure of the molecule. So, that is a very crucial logical information that 1 has used for deducing the structure. I hope you enjoyed this session.

Thank you very much for your attention.